

Nuclide Mixtures

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Why mixtures ?

Mixture vs. simple nuclide → in the real life: mainly mixtures

Often-used module in other applications

Nuclide Mixtures

- User interface

My Mixtures

Wiki help

Edit

Create

Rescale

Import

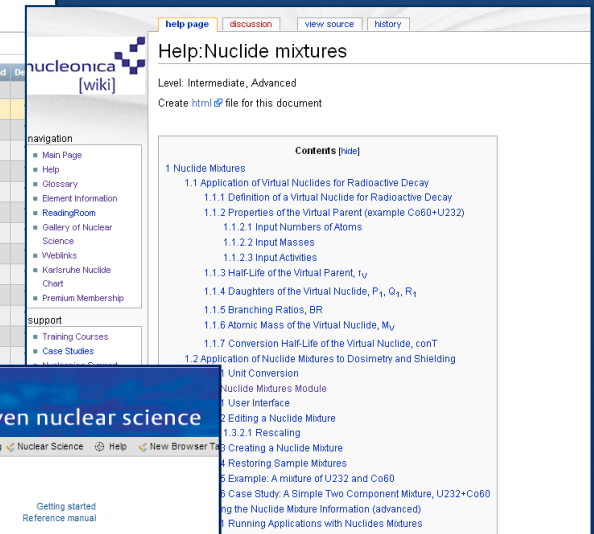
Sample Mixtures

Download

Send mixture(s) to contact

- Abundance and Enrichment

- Exercises

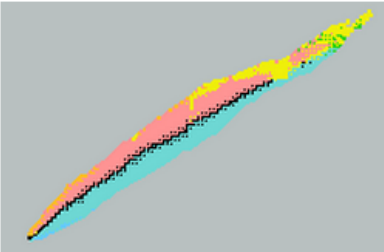


Go to Nuclide Mixtures Application...

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Nuclide Explorer



» Actual Chart: Karlsruhe

Search Nucleonica Documentation

Search

Nuclide Search / Radiation Search

Application Centre

- » **New:** Mass Activity Converter
- » Mass Activity Calculator
- » **New:** Decay Engine++
- » Decay Engine
- » **New:** Dosimetry & Shielding++
- » Dosimetry & Shielding
- » Range & Stopping Power
- » In Silico Dosimetry
- » webKORIGEN
- » Decay Engine for Large Nuclide Sets
- » Universal Nuclide Chart
- » **New:** e-Ship++: radiological transport assistant
- » ~~Old:~~ e-Ship
- » **Transport & Packaging**
- » **Nuclide Mixtures**
- » Nucleonica Scripting
- » Radiological Dispersion Module
- » Gamma Spectrum Generator
- » Gamma Spectrum Generator Pro
- » Virtual Cloud Chamber
- » Geant4 Dosimetry
- » easy Monte Carlo
- » Cambio file Converter
- » **New:** WESPA
- » WESPA1
- » Gamma Library
- » webGraph

Welcome,

My Settings Administration

My Applications

- Mass Activity Converter
- Nuclide Datasheet
- Decay Engine++
- Dosimetry & Shielding++
- e-Ship++: radiological transport assistant

My Last Nuclides

- 27 Co60
- 84 Po218
- 95 Am241
- 82 Pb206
- 82 Pb207 m

My Nuclide Mixtures

- Juelich file 65
- Juelich file 30
- Juelich file 20
- Juelich file 40
- Juelich file 50

My Sources / Packages

- UOX, 1g, Ca137+Am241
- TOF13504.TXT
- Decayed: R-Pu
- R-Pu
- Decayed: Pu-241

My Mixtures

Nuclide mixtures in
bold are Sample
Mixtures

Other mixtures are
user created

To edit click on
mixture...

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Nuclide Mixtures

Getting started
Reference manual

My Mixtures Edit Import Sample Mixtures

User defined nuclide mixtures

Send	Mixture	Date modified ▼	Download	Delete
	(create, upload a new Mixture)			
<input type="checkbox"/>	Natural Potassium	23.10.2012, 13:31:19		
<input type="checkbox"/>	Zircaloy-4	10.09.2012, 19:14:17		
<input type="checkbox"/>	Fukushima spectrum	22.05.2012, 16:35:01		
<input type="checkbox"/>	Decay of 1e6 Becquerel of 58 Ce 144 after 7.80E+00 Years(1E-02)	02.04.2012, 13:50:09		
<input type="checkbox"/>	Cs137 in equilibrium with Ba137m	11.03.2012, 11:59:42		
<input type="checkbox"/>	HEU, highly enriched uranium	06.05.2011, 13:32:54		
<input type="checkbox"/>	Decay of 1.00E+00 Grams of U232+Co60 after 5.26E+01 Years(1.47E-02)	02.03.2011, 10:28:58		
<input type="checkbox"/>	Rb-81/Kr-81m Generator	06.01.2011, 17:03:59		
<input type="checkbox"/>	U element	12.04.2010, 09:57:24		
<input type="checkbox"/>	Natural Uranium	08.04.2010, 15:50:06		
<input type="checkbox"/>	Transuranics in 1 ton Spent Fuel	12.03.2010, 13:00:55		
<input type="checkbox"/>	U232+Co60	10.03.2010, 13:50:08		
<input type="checkbox"/>	Natural Thorium	10.03.2010, 13:36:26		
	All Mixtures (13)			

Send to my contacts:

Nuclide mixtures

Wiki page (Help)

Full technical
documentation

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Help:Nuclide mixtures

Level: Intermediate, Advanced

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 - 1.1.2.1 Input Numbers of Atoms
 - 1.1.2.2 Input Masses
 - 1.1.2.3 Input Activities
 - 1.1.3 Half-Life of the Virtual Parent, t_V
 - 1.1.4 Daughters of the Virtual Nuclide, P_1 , Q_1 , R_1
 - 1.1.5 Branching Ratios, BR
 - 1.1.6 Atomic Mass of the Virtual Nuclide, M_V
 - 1.1.7 Conversion Half-Life of the Virtual Nuclide, $conT$
 - 1.2 Application of Nuclide Mixtures to Dosimetry and Shielding
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 - 1.3.6 Case Study: A Simple Two Component Mixture, U232+Co60
 - 1.4 Storing the Nuclide Mixture Information (advanced)
 - 1.4.1 Running Applications with Nuclides Mixtures

Nuclide Mixtures


In this chapter the formalism for calculations on mixtures of nuclides is developed. In particular the formalism for the radioactive decay of nuclide mixtures. A virtual parent is defined which decays on a time-scale required mixture. The procedure for obtaining the half-life, the daughters, the branching ratios,

nucleonica

Edit

Nuclide Mixture
example:
natural uranium

Version: 2013.10.29 18:



Nuclide Mixtures

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Name

Description:

Nuclide ▲	Activity(Bq)	Mass(g)	Number of Atoms	Mole (atoms)	Activity ratio	Mass ratio	Mole ratio	Delete
(add a new Nuclide, add a new Element)								
92 U 234	2.907e+5	0.01264	3.252e+19	5.400e-5	0.4860	5.310e-5	5.400e-5	
92 U 235	1.354e+5	1.693	4.338e+21	7.204e-3	0.02264	7.114e-3	7.204e-3	
92 U 238	2.939e+6	236.3	5.978e+23	0.9927	0.4913	0.9928	0.9927	
Total: 3	5.981e+6	238.0	6.022e+23	1.000	1	1.000	1	

Element

Mass

Quantity

Unit

U

238

236.3

Gram

Update

Save Mixture

Reset

Cancel

Becquerel

Curie

Number of Atoms

Mole (atoms)

Significant figures:

Click on **Total:...** to rescale the mixture.

Create
a new mixture:

... web driven nuclear science

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Nuclide Mixtures

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My MixturesEditImportSample Mixtures

User defined nuclide mixtures

Send	Mixture	Date modified ▼	Download	Delete
	(create, upload a new mixture)			
	Natural Potassium	23.10.2012, 13:31:19		
	Zircaloy-4	10.09.2012, 19:14:17		
	Fukushima spectrum	22.05.2012, 16:35:01		
	Decay of 1e6 Becquerel of 58 Ce 144 after 7.80E+00 Years(1E-02)	02.04.2012, 13:50:09		
	Cs137 in equilibrium with Ba137m	11.03.2012, 11:59:42		
	HEU, highly enriched uranium	06.05.2011, 13:32:54		
	Decay of 1.00E+00 Grams of U232+Co60 after 5.26E+01 Years(1.47E-02)	02.03.2011, 10:28:58		
	Rb-81/Kr-81m Generator	06.01.2011, 17:03:59		
	U element	12.04.2010, 09:57:24		
	Natural Uranium	08.04.2010, 15:50:06		
	Transuranics in 1 ton Spent Fuel	12.03.2010, 13:00:55		
	U232+Co60	10.03.2010, 13:50:08		
	Natural Thorium	10.03.2010, 13:36:26		
	All Mixtures (13)			

Send to my contacts:


Create a new mixture:

Details

1. In Edit tab, enter a **name** for the mixture
2. Enter short description
3. Enter components → „(add a new nuclide)“
 - Choose a nuclide
 - Select a unit
 - Enter the quantity
 - Update grid
4. Save the mixture

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 **Nuclide Mixtures** [Getting started](#) [Reference manual](#)

My Mixtures Edit Import Sample Mixtures


Name
my highly enriched uranium, HEU

Description:
isotopic composition: 0.77% U-234, 90.20% U-235, 0.33% U-236 and 8.7% U-238.

Nuclide	Activity(Bq)	Mass(g)	Number of Atoms	Mole (atoms)	Activity ratio	Mass ratio	Mole ratio	Delete
92 U 238	1.095e+6	88.02	2.227e+23	0.3698	1	1	1	
Total: 1	1.095e+6	88.02	2.227e+23	0.3698	1	1	1	

(add a new Nuclide, add a new Element)

Element Mass Quantity Unit

U 235 901.0 Gram  Update

Create a new mixture:

Details

My Mixtures Edit Import Sample Mixtures

Name

My highly enriched uranium, HEU

Description:

isotopic composition: 0.77% U-234, 90.20% U-235, 0.33% U-236 and 8.7% U-238.

Nuclide	Activity(Bq)	Mass(g)	Number of Atoms	Mole (atoms)	Activity ratio	Mass ratio	Mole ratio	Delete
<i>(add a new Nuclide, add a new Element)</i>								
92 U 234	1.762e+9	7.659	1.971e+22	0.03272	0.9561	7.659e-3	7.700e-3	
92 U 235	7.205e+7	901.0	2.309e+24	3.833	0.03910	0.9010	0.902	
92 U 236	7.827e+6	3.310	8.446e+21	0.01402	4.248e-3	3.310e-3	3.300e-3	
92 U 238	1.095e+6	88.02	2.227e+23	0.3697	5.940e-4	0.08802	0.08700	
Total: 4	1.843e+9	1.000e+3	2.559e+24	4.250	1	1.000	1	

Element Mass Quantity Unit

U 238 88.02 Gram Update

Save Mixture Reset Cancel

Significant figures: 4

Click on **Total:...** to rescale the mixture.



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My Mixtures Edit Upload Sample Mixtures

Name

HEU, highly enriched uranium

Description:

isotopic composition: 0.77% U-234, 90.20% U-235, 0.33% U-236 and 8.7% U-238.

Nuclide ▲	Activity(Bq)	Mass(g)	Number of Atoms	Mass ratio	Mole ratio	Activity ratio	Delete
(add a new Nuclide)							
92 U 234	6.88347e-14	2.99248e-22	0.770000	7.65876e-3	0.0077	0.956060	
92 U 235	2.81501e-15	3.52050e-20	90.2000	0.901014	0.902000	0.0390983	
92 U 236	3.05835e-16	1.29348e-22	0.330000	3.31044e-3	3.30000e-3	4.24781e-3	
92 U 238	4.27690e-17	3.43905e-21	8.70000	0.0880167	0.087	5.94028e-4	
Total: 4	7.19983e-14	3.90727e-20	100.000	1.00000	1.00000	1	

Element

Mass

Quantity

Unit

1e3

Gram

Update

Save Mixture

Reset

Cancel

Gram
Gram
Becquerel
Curie
Number of Atoms
Mole

Save as Sample

Rescale feature...

Rescale results

for example

from 100 atoms to 1 kg!

Import a new mixture:

Allowed File Formats

Description of format in 1st line:

- Nuclide, Activity (Bq)
- Nuclide, Activity (Ci)
- Nuclide, Mass(g)
- Nuclide, Atoms
- Nuclide, Moles

For the nuclide, the following formats are allowed:

- Co60, (no blank between the element symbol and the isotope)
- Cs 137, (with blank),
- I-123, (with hyphen)
- Tc-99m, (with hyphen and metastable state)

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My Mixtures Edit **Import** Sample Mixtures

Browse a file to be uploaded:

Datei auswählen Keine ausgewählt

Upload File Reset

Import / Upload files:

- CSV: CSV: consisting of rows with (see example file or see File Formats)
 - Nuclide name (e.g.: Co-60), Quantity (in Bq, Ci, g, mole, or atoms)
- XML: special format of previously downloaded Nuclide Mixtures

Decimal separator

☒ Period 1/2 = 0.5

☐ Comma 1/2 = 0,5


Example of CSV file to be imported showing some allowed formats for the nuclide e.g. Co60, Cs 137, I-123.
The first line describes the import data format e.g. Nuclide, Activity(Bq); Nuclide, Mass(g); Nuclide, Activity(Ci); Nuclide, Atoms; Nuclide, Mole

Nuclide,	Activity (Bq)
Co60,	1.5e6
Cs 137,	1000
I-123,	20000
Tc-99m,	3.7e10

Some typical running times

- Nuclides = **30**,
- Mass Activity Converter **<1s**
- Decay Engine++ **10s**
- Dosimetry & Shielding++ **17s (no daughters), 20s (with daughters)**
- Gamma Spectrum Generator **80s**
- Cambio File Converter **<5s**
- WESPA **<7s**

Sample Mixtures: Pre-defined Mixtures



Nuclide Mixtures

My Mixtures Edit Upload Sample Mixtures

Select	Sample Mixture Name	Date Modified	Delete
<input checked="" type="checkbox"/>	Ce-144 / Pr-144	02.04.2012, 14:06:35	
<input checked="" type="checkbox"/>	Cs137 / Ba137m	02.04.2012, 14:07:29	
<input checked="" type="checkbox"/>	Fukushima spectrum	22.05.2012, 16:35:01	
<input checked="" type="checkbox"/>	HEU, highly enriched uranium	06.05.2011, 13:32:54	
<input checked="" type="checkbox"/>	U131_Cs137_mixture	14.03.2011, 16:22:45	
<input checked="" type="checkbox"/>	Natural Thorium	10.03.2010, 13:36:26	
<input checked="" type="checkbox"/>	Natural Uranium	08.04.2010, 15:50:06	
<input checked="" type="checkbox"/>	Rb-81/Kr-81m Generator	06.01.2011, 17:03:59	
<input checked="" type="checkbox"/>	Reactor Grade Pu Sample	10.05.2011, 13:33:12	
<input checked="" type="checkbox"/>	Sr-90 / Y-90	29.03.2012, 14:51:09	
<input checked="" type="checkbox"/>	Transuranics in 1 ton Spent Fuel	10.03.2010, 14:31:18	
<input checked="" type="checkbox"/>	U232+Co60	10.03.2010, 13:50:08	

Send to My Mixtures

Create a new mixture: Save & Download mixture

My Mixtures Edit Upload Sample Mixtures

Name
my highly enriched uranium, HEU

Description:
isotopic composition: 0.77% U-234, 90.20% U-235, 0.33% U-236 and





















Nuclide ▲	Activity(Bq)	Mass(g)	Number of Atoms	Mass ratio	Mol
(add a new Nuclide)					
92 U 234	1.762e+6	7.659e-3	1.971e+19	7.659e-3	7.7
92 U 235	7.205e+4	0.9010	2.309e+21	0.9010	0.902
92 U 236	7.827e+3	3.310e-3	8.446e+18	3.310e-3	4.248e-3
92 U 238	1.095e+3	0.08802	2.227e+20	0.08802	5.940e-4
Total: 4	1.843e+6	1	2.559e+21	1	1

Element Mass Quantity Unit

Save Mixture

My Mixtures Edit Upload Sample Mixtures

User defined nuclide mixtures

Mixture	Date modified ▼	Download	Delete
(create, upload a new Mixture)			
my highly enriched uranium, HEU	06.05.2011, 14:11:37		
HEU, highly enriched uranium	06.05.2011, 13:32:54		
My Uranium	24.02.2011, 17:27:41		
My U232+Co60 Mixture	14.04.2010, 11:04:27		
Natural Uranium	09.04.2010, 14:13:22		
Decay of 1 Grams of 37 Rb 81 after 10 Hours	09.04.2010, 10:43:21		
U232+Co60	10.03.2010, 13:50:08		
Transuranics in 1 ton Spent Fuel	10.03.2010, 14:31:18		
Natural Thorium	10.03.2010, 13:36:26		
Cs137 + Ba137			
All Mixtures (10)			

File Download

Save As

Save in: Mixtures

Mixture_my highly enriched uranium, HEU.xml
Mixture_Natural Uranium.xml
Mixture_UO2 six.xml
Mixture_UO2 with 3 oxygen isotopes.xml
Mixtures_All(2).xml
Mixtures_All(3).xml
Mixtures_All.xml
Mixtures_All_rdf.xml

File name: Mixture_my highly enriched uranium, HEU.xml

Save

Send a Nuclide Mixture to a colleague

There are two possibilities to do this:

1. Download an already existing mixture to your PC. Send this mixture as an email attachment to your colleague. The colleague will have to store this mixtures on his/her PC and then upload it to the Nuclide Mixtures.


2. Use the *Send to my contacts* feature (described here) in the Nuclide Mixtures:

- (a) Tick the check boxes for the mixture(s) to be sent (assume mixture(s) has already been created).
- (b) In the *Send to my contacts*, select the contact from the drop-down list (assume contact already exists in My Contacts)















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 **Nuclide Mixtures** [Getting started](#) [Reference manual](#)

Mixtures Edit Import Sample Mixtures

User defined nuclide mixtures

Send	Mixture	Date modified	Download	Delete
	(create, upload a new Mixture)			
<input checked="" type="checkbox"/>	Cs-137 in equilibrium with Ba-137m	11.03.2012, 11:59:42		
<input checked="" type="checkbox"/>	Decay of 1.00E+00 Grams of U232+Co60 after 5.26E+01 Years(1.47E-02)	02.03.2011, 10:28:58		
<input checked="" type="checkbox"/>	Decay of 1e6 Becquerel of 58 Ce-144 after 7.80E+00 Years(1E-02)	02.04.2012, 13:50:09		
<input type="checkbox"/>	Fukushima spectrum	22.05.2012, 16:35:01		
<input type="checkbox"/>	HEU, highly enriched uranium	06.05.2011, 13:32:54		
<input type="checkbox"/>	M, highly enriched uranium, HEU	30.10.2013, 16:17:24		
<input type="checkbox"/>	Natural Potassium	23.10.2012, 13:31:19		
<input type="checkbox"/>	Natural Thorium	10.03.2010, 13:36:26		
<input type="checkbox"/>	Natural Uranium	08.04.2010, 15:50:06		
<input type="checkbox"/>	Rb-81/Kr-81m Generator	06.01.2011, 17:03:59		
<input type="checkbox"/>	Transuranics in 1 ton Spent Fuel	12.03.2010, 13:00:55		
<input type="checkbox"/>	U element	12.04.2010, 09:57:24		
<input type="checkbox"/>	U232+Co60	10.03.2010, 13:50:08		
<input type="checkbox"/>	Zircaloy-4	10.09.2012, 19:14:17		
	All Mixtures (14)			

Send to my contacts: 

Abundance and Enrichment

The quantities abundance and enrichment are often confused. Whereas the abundance refers to a fraction of the **number** of atoms or atom percent, the enrichment refers to mass. The abundancies are given, for example, in the Karlsruhe Nuclide Chart and in Nucleonica.

O 16	O 17	O 18
99.757	0.038	0.205
σ 0.00019	σ 0.00054 $\sigma_{n,\alpha}$ 0.257	σ 0.00016

Abundance:

The isotopic abundance of an isotope is the fraction of the atoms in the element of that isotope. Isotopic abundancies are usually expressed in atom %.

Enrichment:

Enrichment is normally used in connection with enriched uranium and refers to masses i.e. uranium containing a greater mass percentage of uranium-235 than 0.72%.

Denoting the masses of uranium isotopes by m_4 (mass U-234), m_5 (mass U-235), and m_8 (mass U-238), the enrichment of U-235 in a uranium sample is defined as:

$$x_5 = m_5 / m_U = m_5 / (m_4 + m_5 + m_8)$$

Exercises:

Creating and Using Nuclide Mixtures in Nucleonica

1. Create a nuclide mixture for natural uranium (metallic):

a) Create a nuclide mixture containing 100 atoms of natural uranium using the isotopic abundancies given in the Karlsruhe Nuclide Chart (KNC) i.e.:


U-238: 99.2742 atoms

U-235: 0.7204 atoms

U-234: 0.0054 atoms

U 234	U 235	U 236	U 237	U 238
0.0054	0.7204			99.2742
$2.455 \cdot 10^5$ a	26 m	120 ns	6.75 d	
$2.455 \cdot 10^5$ a	$7.038 \cdot 10^8$ a	$2.342 \cdot 10^7$ a	β^- 0.2...	$4.468 \cdot 10^9$ a
α 4.775, 4.722..., sf Mg28, Ne, γ (53, 121...) e^- , σ 96, σ_f 0.07	α 4.395..., sf Ne, γ 186... σ 95, σ_f 586	α 4.494 4.445..., sf Mg30, γ (49 113...), e^- σ 5.1	γ 60, 208..., e^- $\sigma \sim 100$ $\sigma_f < 0.35$	α 4.198..., sf $2\beta^-$, γ (50...) e^- , σ 2.7 σ_f 3E-6

b) Rescale the results to 1 kg (click on "Total" in the grid to rescale the results)

Nuclide 	Activity(Bq)	Mass(g)	Number of Atoms	Mole	Activity ratio	Mass ratio	Mole ratio
<i>(add a new Nuclide)</i>							
92 U 234	1.22133e+7	0.0530953	1.36620e+20	2.26863e-4	0.486018	5.30953e-5	5.40000e-5
92 U 235	5.68811e+5	7.11366	1.82262e+22	0.0302652	0.0226354	7.11366e-3	7.20400e-3
92 U 238	1.23472e+7	992.833	2.51164e+24	4.17068	0.491347	0.992833	0.992742
Total: 3	2.51292e+7	1000	2.53000e+24	4.20117	1	1	1.00000

Exercises: Creating and Using Nuclide Mixtures in Nucleonica

2. Create a nuclide mixture for natural uranium dioxide:

a) Create a nuclide mixture containing 100 atoms for uranium oxide using the isotopic abundancies in the KNC i.e.:

U-238: 99.2742 atoms,
U-235: 0.7204 atoms,
U-234: 0.0054 atoms

U 234	U 235	U 236	U 237	U 238
0.0054	0.7204	2.342·10 ⁻⁷	6.75 d	99.2742
2.455·10 ⁵ a	26 m	120 ns	β ⁻ 0.2... γ 60, 208..., e ⁻ σ ~100 σ _f < 0.35	280 ns
α 4.775, 4.722..., sf Mg28, Ne, γ(53, 121...) e ⁻ , σ 96, σ _f 0.07	7.038·10 ⁸ a α 4.395..., sf Ne, γ 186... σ 95, σ _f 586	α 4.494 4.445..., sf Mg30, γ (49 113...), e ⁻ σ 5.1	α 4.198..., sf 2β ⁻ , γ (50...) e ⁻ , σ 2.7 σ _f 3E-6	α 4.268·10 ⁹ a α 4.198..., sf 2β ⁻ , γ (50...) e ⁻ , σ 2.7 σ _f 3E-6

In uranium dioxide (UO₂) for every uranium atom there are two oxygen atoms. Hence add 200 atoms of oxygen with the isotopic abundancies given in the KNC i.e.:

O-16: 99.757 x 2 = 199.514 atoms
O-17: 0.038 x 2 = 0.076 atoms
O-18: 0.205 x 2 = 0.410 atoms

O 16	O 17	O 18
99.757	0.038	0.205
σ 0.00019	σ 0.00054 σ _{n,α} 0.257	σ 0.00016

b) Rescale the results to 3 moles (!) (click on "Total" in the grid to rescale the results)

Nuclide	Activity(Bq)	Mass(g)	Number of Atoms	Mole	Activity ratio	Mass ratio	Mole ratio
(add a new Nuclide)							
92 U 238	2.93898e+6	236.323	5.97843e+23	0.992742	0.491347	0.875181	0.330914
92 U 235	1.35393e+5	1.69326	4.33835e+21	7.20400e-3	0.0226354	6.27068e-3	2.40133e-3
92 U 234	2.90711e+6	0.0126382	3.25196e+19	5.40000e-5	0.486018	4.68034e-5	1.80000e-5
8 O 18	0	0.0737966	2.46908e+21	0.0041	0	2.73293e-4	1.36667e-3
8 O 17	0	0.0129193	4.57683e+20	0.00076	0	4.78445e-5	2.53333e-4
8 O 16	0	31.9121	1.20150e+24	1.99514	0	0.118181	0.665047
Total: 6	5.98148e+6	270.028	1.80664e+24	3.00000	1	1.00000	1.00000

3. Create a nuclide mixture for natural UO_2 by adding elements U and O (rather than nuclides)

nucleonica ... web driven nuclear science

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Nuclide Mixtures

Getting started
Reference manual

My Mixtures Edit Upload Sample Mixtures

Name:

Description:

Nuclide	Activity(Bq)	Mass(g)	Number of Atoms	Mole (atoms)	Activity ratio	Mass ratio	Mole ratio	Delete
(add a new Nuclide, add a new Element)								
8 O 16	0	31.9121	1.20150e+24	1.99514	0	0.118181	0.665047	
8 O 17	0	0.0129193	4.57683e+20	0.00076	0	4.78445e-5	2.53333e-4	
8 O 18	0	0.0737966	2.46908e+21	0.0041	0	2.73293e-4	1.36667e-3	
92 U 234	2.90711e+6	0.0126382	3.25196e+19	5.40000e-5	0.486018	4.68034e-5	1.80000e-5	
92 U 235	1.35393e+5	1.69326	4.33835e+21	7.20400e-3	0.0226354	6.27068e-3	2.40133e-3	
92 U 238	2.93898e+6	236.323	5.97843e+23	0.992742	0.491347	0.875181	0.330914	
Total: 6	5.98148e+6	270.028	1.80664e+24	3.00000	1	1	1	

Nuclide	Activity(Bq)	Mass(g)	Number of Atoms	Mole (atoms)	Activity ratio	Mass ratio	Mole ratio	Delete
(add a new Nuclide, add a new Element)								
8 O	0	31.9988	1.20143e+24	2	0	0.118502	0.666667	
92 U	5.98148e+6	238.029	6.02214e+23	1	1	0.881498	0.333333	
Total: 2	5.98148e+6	270.028	1.80664e+24	3.00000	1	1	1	


Significant figures: 6

Click on Total:... to rescale the mixture.

Element Mass Quantity Unit


Click on new Nuclide or new Element to see nuclides/ elements

4. Create a nuclide mixture for Zirconium Hydride $\text{ZrH}_{1.6}$



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Nuclide Mixtures

My MixturesEditUploadSample Mixtures

Name
ZrH1.6

Description:
created by adding elements of Zr and H

Nuclide	Activity(Bq)	Mass(g)	Number of Atoms	Mole (atoms)	Activity ratio	Mass ratio	Mole ratio	Delete
(add a new Nuclide, add a new Element)								
1 H 1	0	1.61233	9.63432e+23	1.59982	0	0.0173675	0.615314	
1 H 2	0	3.70595e-4	1.10807e+20	1.84000e-4	0	3.99191e-6	7.07692e-5	
40 Zr 90	0	46.2560	3.09839e+23	0.5145	0	0.498253	0.197885	
40 Zr 91	0	10.1996	6.75684e+22	0.1122	0	0.109867	0.0431538	
40 Zr 92	0	15.7617	1.03280e+23	0.1715	0	0.169780	0.0659615	
40 Zr 94	0.383151	16.3209	1.04665e+23	0.1738	0.999975	0.175803	0.0668462	
40 Zr 96	9.49652e-6	2.68543	1.68620e+22	0.028	2.47847e-5	0.0289265	0.0107692	
Total: 7	0.383161	92.8364	1.56576e+24	2.60000	1	1.00000	1.00000	

Nuclide	Activity(Bq)	Mass(g)	Number of Atoms	Mole (atoms)	Activity ratio	Mass ratio	Mole ratio	Delete
(add a new Nuclide, add a new Element)								
1 H	0	1.61271	9.63432e+23	1.6	0	0.0173715	0.615385	
40 Zr	0.383161	91.2236	6.02214e+23	1	1	0.982629	0.384615	
Total: 2	0.383161	92.8364	1.56576e+24	2.6	1	1.00000	1	

Significant figures: 6

Click on Total:... to rescale the mixture.

ElementMassQuantityUnit

1

Mole (atoms)

Update

Save MixtureResetCancelSave as Sample



5. Create a nuclide mixture for Zircaloy-4

Zircaloy-4 mixture: Using the previously described procedure even more complicated mixtures can be created. One such example is Zircaloy-4 (Zyr-4) which is used as a cladding material in nuclear power reactors.

Composition of Zircaloy-4 (gram/kg Zyr-4): H (0.025), B (0.0005), C (0.27), O (1.6), Mg (0.02), Al (0.075), Si (0.12), N (0.065), Ti (0.05), Cr (1.3), Mn (0.05), Fe (2.4), Co (0.02), Ni (0.07), Cu (0.05), Zr (976.559), Mo (0.05), Cd (0.0005), Sn (17), Hf (0.1), W (0.1), U (0.075)

Create a mixture using only the main 5 elements (which accounts for 99.8859 of the mass)

The screenshot shows the Nucleonica software interface. The top part displays a table of nuclides with columns: Nuclide, Activity, Mass(g), Number of Atoms, Mole (atoms), Activity ratio, Mass ratio, Mole ratio, and Delete. A red circle highlights the 'Add a new Nuclide, add a new Element' button. Below this, the 'My Mixtures' section shows a form for naming and describing the mixture. The name is 'Zyr-4 (Zr, Sn, Fe, Cr, O)' and the description is 'use the top 5 elements by mass (gram/kg Zyr-4): O (1.6), Cr (1.3), Fe (2.4), Zr (976.559), Sn (17)'. Below the form, a table shows the composition of the mixture with columns: Nuclide, Activity, Mass(g), Number of Atoms, Mole (atoms), Activity ratio, Mass ratio, Mole ratio, and Delete. A red circle highlights the 'Add a new Nuclide, add a new Element' button. At the bottom, there is a form for creating a mixture with fields for Element, Mass, Quantity, and Unit, and buttons for 'Save Mixture', 'Reset', 'Cancel', and 'Save as Sample'.

Nuclide	Activity	Mass(g)	Number of Atoms	Mole (atoms)	Activity ratio	Mass ratio	Mole ratio	Delete
(add a new Nuclide, add a new Element)								
8 O 16	0	1.59566	6.00773e+22	0.0997607	0	1.59749e-3	9.05574e-3	
8 O 17	0	6.45991e-4	2.28850e+19	3.80014e-5	0	6.46729e-7	3.44956e-6	
8 O 18	0	3.68997e-3	1.23458e+20	2.05008e-4	0	3.69418e-6	1.86095e-5	
24 Cr 50	7.98292e-5	0.0542579	6.54204e+20	1.08633e-3	1.94565e-5	5.43199e-5	9.86113e-5	
24 Cr 52	0	1.08809	1.26157e+22	0.0209488	0	1.08933e-3	1.90162e-3	
24 Cr 53	0	0.125757	1.43052e+21	2.37543e-3	0	1.25900e-4	2.15628e-4	
24 Cr 54	0	0.0318937	3.56086e+20	5.91294e-4	0	3.19302e-5	5.36745e-5	
26 Fe 54	0	0.135493	1.51273e+21	2.51195e-3	0	1.35648e-4	2.28021e-4	
26 Fe 56	0	2.20564	2.37466e+22	0.0394322	0	2.20816e-3	3.57944e-3	
26 Fe 57	0	0.0518488	5.48413e+20	9.10661e-4	0	5.19081e-5	8.26649e-5	
26 Fe 58	0	7.02107e-3	7.29837e+19	1.21192e-4	0	7.02909e-6	1.10012e-5	
40 Zr 90	0	495.175	3.31686e+24	5.50778	0	0.495741	0.499966	
40 Zr 91	0	109.188	7.23327e+23	1.20111	0	0.109313	0.109031	
40 Zr 92	0	168.731	1.10562e+24	1.83593	0	0.168924	0.166655	
40 Zr 94	4.10167	174.717	1.12045e+24	1.86055	0.999688	0.174917	0.168891	
40 Zr 96	1.01661e-4	28.7478	1.80509e+23	0.299743	2.47776e-5	0.0287807	0.0272091	
50 Sn 112	0	0.155447	8.36535e+20	1.38910e-3	0	1.55624e-4	1.26095e-4	
50 Sn 114	0	0.107656	5.69189e+20	9.45160e-4	0	1.07779e-4	8.57965e-5	
50 Sn 115	0	0.0559465	2.93218e+20	4.86900e-4	0	5.60104e-5	4.41982e-5	
50 Sn 116	0	2.41332	1.25394e+22	0.0208222	0	2.41608e-3	1.89012e-3	
50 Sn 117	0	1.28572	6.62328e+21	0.0109982	0	1.28719e-3	9.98359e-4	
50 Sn 118	0	4.08936	2.08875e+22	0.0346845	0	4.09403e-3	3.14847e-3	
50 Sn 119	0	1.46268	7.40807e+21	0.0123014	0	1.46435e-3	1.11665e-3	
50 Sn 120	0	5.59422	2.80972e+22	0.0466565	0	5.60061e-3	4.23523e-3	
50 Sn 122	0	0.808273	3.99294e+21	6.63044e-3	0	8.09196e-4	6.01875e-4	
50 Sn 124	1.09676e-3	1.02738	4.99334e+21	8.29163e-3	2.67310e-4	1.02855e-3	7.52669e-4	
Total: 26	4.10295	998.859	6.63417e+24	11.0163	1	1.00000	1.00000	

Name: Zyr-4 (Zr, Sn, Fe, Cr, O)

Description: use the top 5 elements by mass (gram/kg Zyr-4):
O (1.6), Cr (1.3), Fe (2.4), Zr (976.559), Sn (17)

Nuclide	Activity	Mass(g)	Number of Atoms	Mole (atoms)	Activity ratio	Mass ratio	Mole ratio	Delete
(add a new Nuclide, add a new Element)								
8 O	0	1.60000	6.02217e+22	0.100004	0	1.60183e-3	9.07780e-3	
24 Cr	7.98292e-5	1.3	1.50565e+22	0.0250019	1.94565e-5	1.30148e-3	2.26953e-3	
26 Fe	0	2.40000	2.58807e+22	0.0429760	0	2.40274e-3	3.90113e-3	
40 Zr	4.10178	976.559	6.44677e+24	10.7051	0.999713	0.977675	0.971752	
50 Sn	1.09676e-3	17.0000	8.62407e+22	0.143206	2.67310e-4	0.0170194	0.0129995	
Total: 5	4.10295	998.859	6.63417e+24	11.0163	1	1	1.00000	

Element: [dropdown] Mass: [dropdown] Quantity: 1 Unit: Gram [dropdown] [Update]

[Save Mixture] [Reset] [Cancel] [Save as Sample]

Exercises: Creating and Using Nuclide Mixtures in Nucleonica

6. Create a nuclide mixture for enriched uranium (metallic) where the U-235 enrichment is 4% (include U-234 in the calculation).

Denoting the masses of uranium isotopes by m_4 (mass U-234), m_5 (mass U-235), and m_8 (mass U-238), the enrichment of U-235, x_5 , in a uranium sample is defined as:

$$x_5 = m_5 / m_U = m_5 / (m_4 + m_5 + m_8)$$

In enriched uranium, assume the ratio of masses m_4/m_5 same as in natural U i.e.

$$m_4/m_5 = 2.099\text{e-}24/2.812\text{e-}22 = 7.46\text{e-}3 \text{ (see Appendix)}$$

$$\rightarrow m_4 = 7.46\text{e-}3 * m_5$$


$$m_5 = x_5 * m_8 / (1 - x_5 * 1.00746)$$

For $x = 0.04$, $m_8 = 100$ g:

$$m_5 = 4 / 0.9597 = 4.168 \text{ g,}$$

$$m_4 = 7.46\text{e-}3 * m_5 = 3.109\text{e-}2 \text{ g}$$

Now rescale to 100 g

Nuclide 	Activity(Bq)	Mass(g)	Number of Atoms	Mole	Activity ratio	Mass ratio	Mole ratio
<i>(add a new Nuclide)</i>							
92 U 234	6.863e+6	0.02984	7.677e+19	1.275e-4	0.8193	2.984e-4	3.033e-4
92 U 235	3.198e+5	4.000	1.025e+22	0.01702	0.03818	0.04000	0.04049
92 U 238	1.194e+6	95.97	2.428e+23	0.4031	0.1425	0.9597	0.9592
Total: 3	8.377e+6	100.0	2.531e+23	0.4203	1	1	1

Exercises: Creating and Using Nuclide Mixtures in Nucleonica

7. Create a nuclide mixture for enriched uranium dioxide where the U-235 enrichment is 4% (include U-234 and oxygen isotopes in the calculation).

a) Start with the nuclide mixtures for 100 g 4% enriched uranium i.e.

Nuclide ▲	Activity(Bq)	Mass(g)	Number of Atoms	Mole	Activity ratio	Mass ratio	Mole ratio
(add a new Nuclide)							
92 U 234	6.863e+6	0.02984	7.677e+19	1.275e-4	0.8193	2.984e-4	3.033e-4
92 U 235	3.198e+5	4.000	1.025e+22	0.01702	0.03818	0.04000	0.04049
92 U 238	1.194e+6	95.97	2.428e+23	0.4031	0.1425	0.9597	0.9592
Total: 3	8.377e+6	100.0	2.531e+23	0.4203	1	1	1

b) In a second step, rescale the mixture to 100 atoms, i.e.

Nuclide ▲	Activity(Bq)	Mass(g)	Number of Atoms	Mole	Activity ratio	Mass ratio	Mole ratio
(add a new Nuclide)							
92 U 234	2.712e-15	1.179e-23	0.03033	5.037e-26	0.8193	2.984e-4	3.033e-4
92 U 235	1.264e-16	1.580e-21	4.049	6.724e-24	0.03818	0.04000	0.04049
92 U 238	4.715e-16	3.792e-20	95.92	1.593e-22	0.1425	0.9597	0.9592
Total: 3	3.310e-15	3.951e-20	100.0	1.661e-22	1	1	1

c) Now add 200 atoms of oxygen isotopes as in example 2.

Nuclide ▼	Activity(Bq)	Mass(g)	Number of Atoms	Mole (atoms)	Activity ratio	Mass ratio	Mole ratio
(add a new Nuclide, add a new Element)							
92 U 238	4.715e-16	3.792e-20	95.92	1.593e-22	0.1425	0.8459	0.3197
92 U 235	1.264e-16	1.580e-21	4.049	6.724e-24	0.03818	0.03526	0.01350
92 U 234	2.712e-15	1.179e-23	0.03033	5.037e-26	0.8193	2.630e-4	1.011e-4
8 O 18	0	1.225e-23	0.4100	6.808e-25	0	2.734e-4	1.367e-3
8 O 17	0	2.145e-24	0.07600	1.262e-25	0	4.786e-5	2.533e-4
8 O 16	0	5.299e-21	199.5	3.313e-22	0	0.1182	0.6650
Total: 6	3.310e-15	4.482e-20	300	4.982e-22	1	1.000	1.000

Nuclide Mixtures

- User interface

My Mixtures

Wiki help

Edit

Create

Rescale

Import

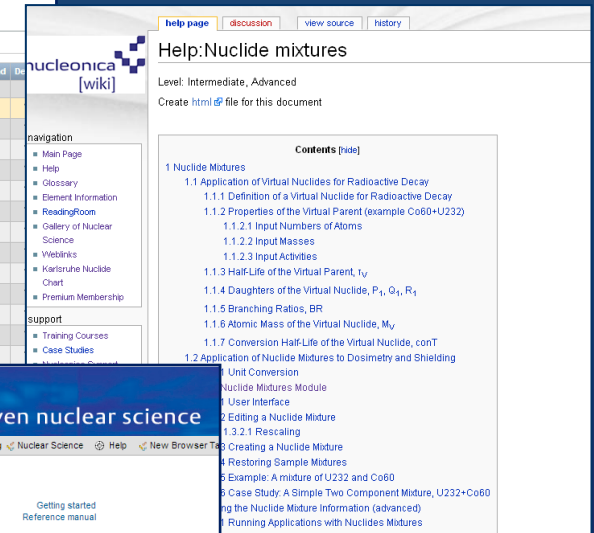
Sample Mixtures

Download

Send mixture(s) to contact

- Abundance and Enrichment

- Exercises



Appendix

$$x_5 = m_5 / m_U = m_5 / (m_4 + m_5 + m_8)$$

In enriched uranium, assume the ratio of masses m_4/m_5 same as in natural U i.e.

$$m_4/m_5 = 2.099\text{e-}24/2.812\text{e-}22 = 7.46\text{e-}3$$

$$\rightarrow m_4 = 7.46\text{e-}3 * m_5$$

$$x_5 = m_5 / (7.46\text{e-}3 * m_5 + m_5 + m_8) = m_5 / (1.00746 * m_5 + m_8)$$

$$m_5 = x_5 * (1.00746 * m_5 + m_8) = x_5 * 1.00746 * m_5 + x_5 * m_8$$

$$m_5 (1 - x_5 * 1.00746) = x_5 * m_8$$

$$\Rightarrow m_5 = x_5 * m_8 / (1 - x_5 * 1.00746)$$

For $x_5 = 0.04$, $m_8 = 100$ g:

$$m_5 = 4 / 0.9597 = 4.168 \text{ g},$$

$$m_4 = 7.46\text{e-}3 * m_5 = 3.109\text{e-}2 \text{ g}$$